Pentane

109-66-0 | DTXSID2025846

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -136 °C

Global applicability domain: Inside

Local applicability domain index: 9.43e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

Image not found

Pentane
Measured: -130
Predicted: -136

Image not found

2-Methylbutane
Measured: -160
Predicted: -119

Image not found

n-Hexane
Measured: -95.3
Predicted: -116

Image not found

3-Methylpentane
Measured: -163
Predicted: -127

Image not found

Butane
Measured: -138
Predicted: -147